Chemistry of Heterocyclic Compounds 1971 vol.4 N4, pages 444-447

Six-membered heterocycles - I. The stereoisomerism of 2-alkyl-5-hexyl-1,3-dioxanes

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Abstract

2-Methyl-5-hexyl- and 2-isopropyl-5-hexyl-1, 3-dioxanes have been synthesized for the first time by the condensation of 2-hexyl-1, 3-propane-diol with acetaldehyde and isobutyraldehyde, and they have been separated into their stereoisomers by fractionation in efficient columns. It has been shown by a study of their PMR spectra that the low-boiling isomers have the cis- and the high-boiling isomers the trans-configuration. A study of the PMR spectra has enabled us to show not only the configuration but also the predominant conformations of the isomers; the cis-isomer exists predominantly in the unsymmetrical boat conformation with a diequatorial location of the substituents and the trans-isomer in the chair conformation, also with a diequatorial arrangement of the substituents.

http://dx.doi.org/10.1007/BF00486752